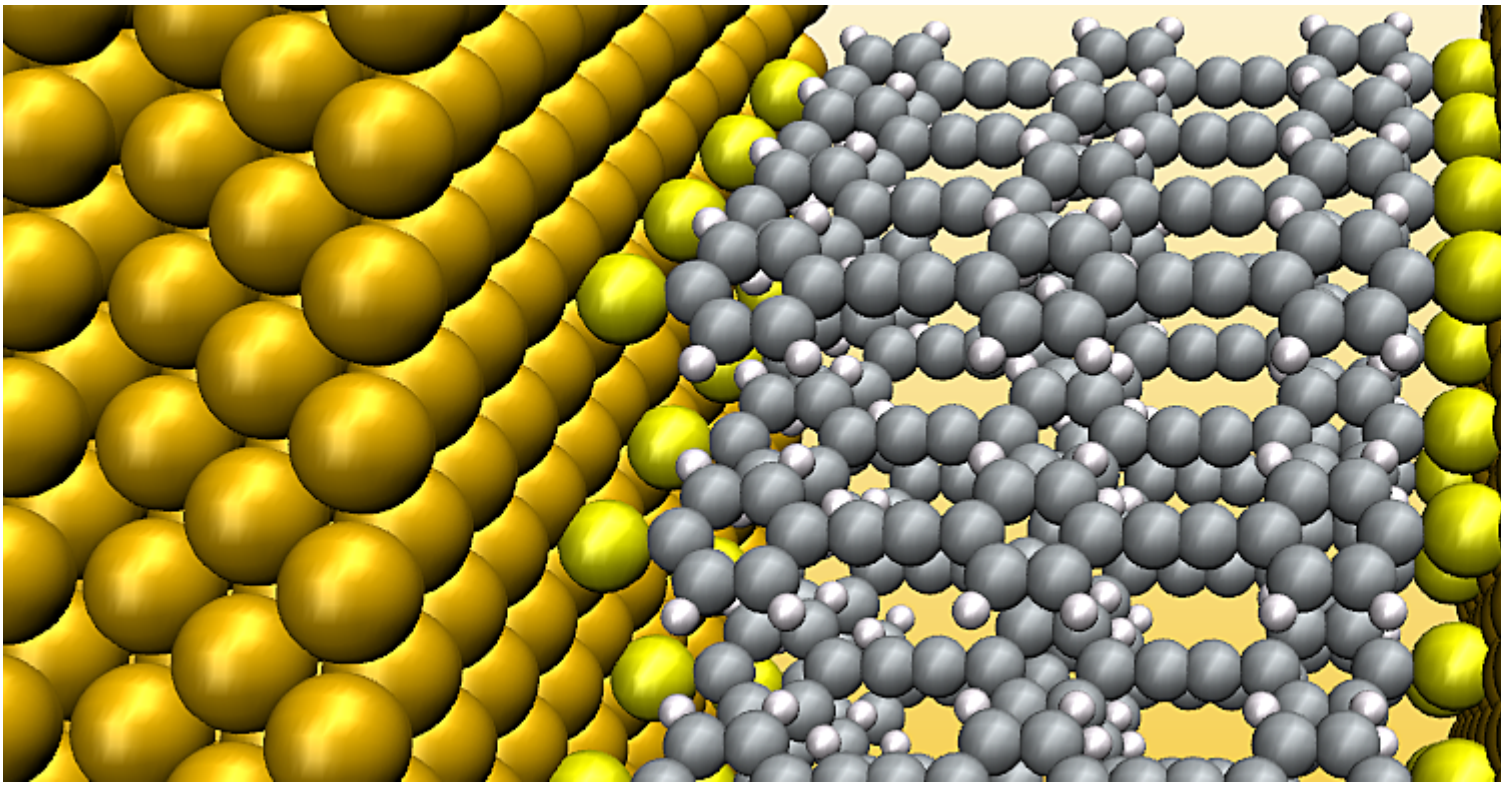
Electronic transport



This research line aims at the development and application of electronic transport simulation tools. We use ab-initio approaches based on fundamental quantum mechanical principles to get highly precise and reliable results.

Summary

We are investigating the electronic transport properties of materials, which is a key factor for many applications. We focus on an atomistic description and employ first-principles techniques and to get precise and unbiased results. The increasing power of nowadays' supercomputers and the continuous effort in developing highly efficient codes have made it possible to study systems at realistic industry-relevant sizes, providing valuable insights into the characteristics of these materials. BSC contributes with HPC-related code development as well as assistance with research on tools of various levels of theory. The main contribution to this is the development of TranSIESTA, a first-principles electronic transport simulation tool based on Non-Equilibrium Green's Functions (NEGF). This work is carried out in close collaboration with the SIESTA code developers at the Catalan Institute of Nanoscience and Nanotechnology (ICN2).

Objectives

- Improving scalability and performance of simulation tools
- Assistance with execution of demanding simulations
- Representation of simulation tools in large projects
- Collaborate in applied research topics

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